#### I Claim:

10

20

30

1. A system of computing and rendering the nature of bound atomic and atomic ionic electrons from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration, comprising:

processing means for processing and solving the equations for charge, mass, and current density functions of electron(s) in a selected atom or ion, wherein the equations are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration; and

a display in communication with the processing means for displaying the current and charge density representation of the electron(s) of the selected atom or ion.

The system of claim 1, wherein the display is at least one of visual or graphical media.

3. The system of claim 1, wherein the display is at least one of static or dynamic.

4. The system of claim 3, wherein the processing means is constructed and arranged so that at least one of spin and orbital angular motion can be displayed.

- 5. The system of claim 1, wherein the processing means is constructed and arranged so that the displayed information can be used to model reactivity and physical properties.
  - 6. The system of claim 1, wherein the processing means is constructed and arranged so that the displayed information can be used to model other atoms and atomic ions and provide utility to anticipate their reactivity and physical properties.
  - 7. The system of claim 1, wherein the processing means is a general purpose computer.
- 35 8. The system of claim 7, wherein the general purpose computer comprises a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or other storage

device, an input means such as a keyboard or mouse, a display device, and a printer or other output device.

- 9. The system of claim 1, wherein the processing means comprises a special purpose computer or other hardware system.
  - 10. The system of claim 1, further comprising computer program products.
- 11. The system of claim 1, further comprising computer readable media having
   embodied therein program code means in communication with the processing means.
  - 12. The system of claim 11, wherein the computer readable media is any available media that can be accessed by a general purpose or special purpose computer.

15

20

- 13. The system of claim 12, wherein the computer readable media comprises at least one of RAM, ROM, EPROM, CD ROM, DVD or other optical disk storage, magnetic disk storage or other magnetic storage devices, or any other medium that can embody a desired program code means and that can be accessed by a general purpose or special purpose computer.
- 14. The system of claim 13, wherein the program code means comprises
  executable instructions and data which cause a general purpose computer or special
  purpose computer to perform a certain function of a group of functions.
  - 15. The system of claim 14, wherein the program code is Mathematica programmed with an algorithm based on the physical solutions.
- 30 16. The system of claim 15, wherein the algorithm for the rendering of the electron of atomic hydrogen using Mathematica is

SphericalPlot3D[1,{q,0,p},{f,0,2p},Boxed®False,Axes®False];

and the algorithm for the rendering of atomic hydrogen using Mathematica and computed on a PC is

Electron=SphericalPlot3D[1,{q,0,p},{f,0,2p-p/2},Boxed®False,Axes®False]; Proton=Show[Graphics3D[{Blue,PointSize[0.03],Point[{0,0,0}]}],Boxed®False]; Show[Electron,Proton];

17. The system of claim 15, wherein the algorithm for the rendering of the spherical-and-time-harmonic-electron-charge-density functions using Mathematica are

5

20

## To generate L1MO;

L1MOcolors[theta\_,phi\_,det\_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],det <.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.533 
3,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,RG 
BColor[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RGB 
Color[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBColor[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.070,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.32 
6,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000];

L1MO=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta] Sin[phi],Cos[theta],L1MOcolors[theta,phi,1+Cos[theta]]},{theta,0,Pi},{phi,0,2Pi},Boxe d®False,Axes®False,Lighting®False,PlotPoints®{20,20},ViewPoint®{-0.273,-2.030,3.494}];

### To generate L1MX;

L1MXcolors[theta\_, phi\_, det\_] = Which[det < 0.1333, RGBColor[1.000, 0.070, 0.079],det < .2666, RGBColor[1.000, 0.369, 0.067],det < .4, RGBColor[1.000, 0.681, 0.049],det < .5333, RGBColor[0.984, 1.000, 0.051], det < .6666, RGBColor[0.673, 1.000, 0.058], det < .8, RGBColor[0.364, 1.000, 0.055],det < .9333, RGBColor[0.071, 1.000, 0.060], det < 1.066, RGBColor[0.085, 1.000, 0.388],det < 1.2, RGBColor[0.070, 1.000, 0.678], det < 1.333, RGBColor[0.070, 1.000, 1.000, 0.678], det < 1.333, RGBColor[0.070, 1.000, 0.678], det < 1.333, RGBColor[0.070, 1.000, 0.055], det < 1.6, RGBColor[0.075, 0.401, 1.000],det < 1.733, RGBColor[0.067, 0.082, 1.000], det < 1.866, RGBColor[0.326, 0.056, 1.000],det <= 2, RGBColor[0.674, 0.079, 1.000]];

### L1MX=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta]

35 Sin[phi],Cos[theta],L1MXcolors[theta,phi,1+Sin[theta]
Cos[phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed@False,Axes@False,Lighting@False,PlotPoint
s@{20,20},ViewPoint@{-0.273,-2.030,3.494}];

## To generate L1MY;

L1MYcolors[theta\_,phi\_,det\_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],det</td>

5
.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.5333</td>

,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,RGB</td>

Color[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RGBC</td>

olor[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBColor[</td>

0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.07</td>

0
5,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.326,</td>

0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];

L1MY=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta] Sin[phi],Cos[theta],L1MYcolors[theta,phi,1+Sin[theta]

15 Sin[phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed®False,Axes®False,Lighting®False,PlotPoint s®{20,20}];

### To generate L2MO;

- 20 L2MOcolors[theta\_, phi\_, det\_] = Which[det < 0.2, RGBColor[1.000, 0.070, 0.079],det < .4, RGBColor[1.000, 0.369, 0.067],det < .6, RGBColor[1.000, 0.681, 0.049],det < .8, RGBColor[0.984, 1.000, 0.051],det < 1, RGBColor[0.673, 1.000, 0.058],det < 1.2, RGBColor[0.364, 1.000, 0.055],det < 1.4, RGBColor[0.071, 1.000, 0.060],det < 1.6, RGBColor[0.085, 1.000, 0.388],det < 1.8, RGBColor[0.070, 1.000, 0.678],det < 2, RGBColor[0.070, 1.000, 1.000],det < 2.2, RGBColor[0.067, 0.698, 1.000],det < 2.4, RGBColor[0.075, 0.401, 1.000],det < 2.6, RGBColor[0.067, 0.082, 1.000],det < 2.8, RGBColor[0.326, 0.056, 1.000],det <= 3, RGBColor[0.674, 0.079, 1.000]];</p>
- L2MO=ParametricPlot3D[{Sin[theta] Cos[phi], Sin[theta] Sin[phi], Cos[theta], L2MOcolors[theta, phi, 3Cos[theta] Cos[theta]]},
   {theta, 0, Pi}, {phi, 0, 2Pi},
   Boxed -> False, Axes -> False, Lighting -> False,
   PlotPoints-> {20, 20},
   ViewPoint->{-0.273, -2.030, 3.494}];

# To generate L2MF;

L2MFcolors[theta\_,phi\_,det\_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],det<
.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.5333
,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,RGB
Color[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RGBC

5 olor[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBColor[
0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.070,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.326,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];

- L2MF=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta] Sin[phi],Cos[theta],L2MFcolors[theta,phi,1+.72618 Sin[theta] Cos[phi] 5 Cos[theta] Cos[theta]-.72618 Sin[theta] Cos[phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed®False,Axes®False,Lighting®False,PlotPoint s®{20,20},ViewPoint®{-0.273,-2.030,2.494}];
- To generate L2MX2Y2;
- L2MX2Y2colors[theta\_,phi\_,det\_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079], det<.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.
  20 5333,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8, RGBColor[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,R GBColor[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGB Color[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.075,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.0326,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];
  - L2MX2Y2=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta] Sin[phi],Cos[theta],L2MX2Y2colors[theta,phi,1+Sin[theta] Sin[theta] Cos[2 phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed®False,Axes®False,Lighting®False,PlotPoints®{ 20,20},ViewPoint®{-0.273,-2.030,3.494}];

### To generate L2MXY;

L2MXYcolors[theta\_,phi\_,det\_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],det<.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.53
33,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,R
GBColor[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RG

BColor[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBColor[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.075,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.326,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];

- ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta] Sin[phi],Cos[theta],L2MXYcolors[theta,phi,1+Sin[theta] Sin[theta] Sin[2 phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed®False,Axes®False,Lighting®False,PlotPoints®{ 20,20},ViewPoint®{-0.273,-2.030,3.494}].
  - 18. The system of claim 1 wherein the physical, Maxwellian solutions of the charge, mass, and current density functions of atoms and atomic ions comprises a solution of the classical wave equation  $\left[\nabla^2 \frac{1}{v^2} \frac{\partial^2}{\partial t^2}\right] \rho(r, \theta, \phi, t) = 0$ .
- 1519. The system of claim 18, wherein the time, radial, and angular solutions of the wave equation are separable.
- 20. The system of claim 18, wherein the boundary constraint of the wave equation solution is nonradiation according to Maxwell's equations.
  - 21. The system of claim 20, wherein a radial function that satisfies the boundary condition is a radial delta function

$$f(r) = \frac{1}{r^2} \delta(r - r_n).$$

22. The system of claim 21, wherein the boundary condition is met for a time harmonic function when the relationship between an allowed radius and the electron wavelength is given by

$$2 \pi r_n = \lambda_n,$$

$$\omega = \frac{\hbar}{m_e r^2}, \text{ and}$$

$$v = \frac{\hbar}{m_e r}$$

10

25

where  $\omega$  is the angular velocity of each point on the electron surface,  $\nu$  is the velocity of each point on the electron surface, and r is the radius of the electron.

35 23. The system of claim 22, wherein the spin function is given by the uniform

function  $Y_0^0(\phi,\theta)$  comprising angular momentum components of  $\mathbf{L}_{xy}=\frac{\hbar}{4}$  and  $\mathbf{L}_z=\frac{\hbar}{2}$ .

24. The system of claim 23, wherein the atomic and atomic ionic charge and current density functions of bound electrons are described by a charge-density (mass-density) function which is the product of a radial delta function, two angular functions (spherical harmonic functions), and a time harmonic function:

 $\rho(r,\theta,\phi,t) = f(r)A(\theta,\phi,t) = \frac{1}{r^2}\delta(r-r_n)A(\theta,\phi,t); \qquad A(\theta,\phi,t) = Y(\theta,\phi)k(t)$ 

wherein the spherical harmonic functions correspond to a traveling charge density
wave confined to the spherical shell which gives rise to the phenomenon of orbital
angular momentum.

25. The system of claim 24, wherein based on the radial solution, the angular charge and current-density functions of the electron,  $A(\theta, \phi, t)$ , must be a solution of the wave equation in two dimensions (plus time),

 $\left[\nabla^2 - \frac{1}{v^2} \frac{\partial^2}{\partial t^2}\right] A(\theta, \phi, t) = 0$ 

where  $\rho(r,\theta,\phi,t) = f(r)A(\theta,\phi,t) = \frac{1}{r^2}\delta(r-r_n)A(\theta,\phi,t)$  and  $A(\theta,\phi,t) = Y(\theta,\phi)k(t)$   $\left[\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)_{r,\phi} + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)_{r,\phi} - \frac{1}{v^2}\frac{\partial^2}{\partial^2}\right]A(\theta,\phi,t) = 0$ 

where  $\bar{\nu}$  is the linear velocity of the electron.

26. The system of claim 25, wherein the charge-density functions including the time-function factor are

 $\Omega = 0$ 

20

25

 $\rho(r,\theta,\phi,t) = \frac{e}{8\pi r^2} \left[ \delta(r-r_n) \right] \left[ Y_0^0(\theta,\phi) + Y_\ell^m(\theta,\phi) \right]$ 

J ≠0

30  $\rho(r,\theta,\phi,t) = \frac{e}{4\pi r^2} \left[ \delta(r-r_n) \right] \left[ Y_0^0(\theta,\phi) + \operatorname{Re} \left\{ Y_\ell^m(\theta,\phi) e^{i\omega_n t} \right\} \right]$ 

where  $Y_{\ell}^{m}(\theta,\phi)$  are the spherical harmonic functions that spin about the z-axis with angular frequency  $\omega_n$  with  $Y_0^0(\theta,\phi)$  the constant function

Re  $\{Y_{\ell}^{m}(\theta,\phi)e^{i\omega_{\ell}t}\}=P_{\ell}^{m}(\cos\theta)\cos(m\phi+\omega_{n}t)$  where to keep the form of the spherical harmonic as a traveling wave about the z-axis,  $\omega_{n}=m\omega_{n}$ .

- 27. The system of claim 26, wherein the spin and angular moment of inertia, I,

$$I_z = I_{spin} = \frac{m r_n^2}{2}$$
$$L_z = I\omega \mathbf{i}_z = \pm \frac{\hbar}{2}$$

$$E_{rotational} = E_{rotational, spin} = \frac{1}{2} \left[ I_{spin} \left( \frac{\hbar}{m_e r_n^2} \right)^2 \right] = \frac{1}{2} \left[ \frac{m_e r_n^2}{2} \left( \frac{\hbar}{m_e r_n^2} \right)^2 \right] = \frac{1}{4} \left[ \frac{\hbar^2}{2 I_{spin}} \right]$$

20

$$I_{orbital} = m_{e} r_{n}^{2} \left[ \frac{\ell(\ell+1)}{\ell^{2} + \ell + 1} \right]^{\frac{1}{2}}$$

$$L_{z} = m\hbar$$

$$L_{z total} = L_{z spin} + L_{z orbital}$$

$$E_{rotational, orbital} = \frac{\hbar^{2}}{2I} \left[ \frac{\ell(\ell+1)}{\ell^{2} + 2\ell + 1} \right]$$

$$T = \frac{\hbar^{2}}{2m_{e} r_{n}^{2}}$$

$$\langle E_{rotational, orbital} \rangle = 0.$$

28. The system of claim 1, wherein the force balance equation for one-electron atoms and ions is

$$\frac{m_e}{4\pi r_1^2} \frac{v_1^2}{r_1} = \frac{e}{4\pi r_1^2} \frac{Ze}{4\pi \varepsilon_o r_1^2} - \frac{1}{4\pi r_1^2} \frac{\hbar^2}{m_p r_n^3}$$

$$r_1 = \frac{a_H}{Z}$$

- 25 where  $a_H$  is the radius of the hydrogen atom.
  - 29. The system of claim 28, wherein from Maxwell's equations, the potential energy V, kinetic energy T, electric energy or binding energy  $E_{ele}$  are

$$V = \frac{-Ze^{2}}{4\pi\varepsilon_{o}r_{1}} = \frac{-Z^{2}e^{2}}{4\pi\varepsilon_{o}a_{H}} = -Z^{2}X \ 4.3675 \ X \ 10^{-18} \ J = -Z^{2}X \ 27.2 \ eV$$

$$T = \frac{Z^{2}e^{2}}{8\pi\varepsilon_{o}a_{H}} = Z^{2}X \ 13.59 \ eV$$

$$T = E_{ele} = -\frac{1}{2}\varepsilon_{o} \int_{-\infty}^{r_{1}} \mathbf{E}^{2}dv \quad \text{where } \mathbf{E} = -\frac{Ze}{4\pi\varepsilon_{o}r^{2}}$$

$$E_{ele} = -\frac{Z^2 e^2}{8\pi\varepsilon_o a_H} = -Z^2 X 2.1786 \ X \, 10^{-18} \ J = -Z^2 X 13.598 \ eV.$$

30. The system of claim 1, wherein the force balance equation solution of two electron atoms is a central force balance equation with the nonradiation condition given by

$$\frac{m_e}{4\pi r_2^2} \frac{v_2^2}{r_2} = \frac{e}{4\pi r_2^2} \frac{(Z-1)e}{4\pi \varepsilon_0 r_2^2} + \frac{1}{4\pi r_2^2} \frac{\hbar^2}{Zm_e r_2^3} \sqrt{s(s+1)}$$

which gives the radius of both electrons as

$$r_2 = r_1 = a_0 \left( \frac{1}{Z-1} - \frac{\sqrt{s(s+1)}}{Z(Z-1)} \right); s = \frac{1}{2}.$$

10 31. The system of claim 30, wherein the ionization energy for helium, which has no electric field beyond  $r_1$  is given by

Ionization Energy(He) = -E(electric) + E(magnetic) where,

$$E(electric) = -\frac{(Z-1)e^2}{8\pi\varepsilon_o r_1}$$

$$E(magnetic) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r_1^3}$$

For  $3 \le Z$ 

15

25

Ionization Energy = -Electric Energy -  $\frac{1}{7}$  Magnetic Energy.

- 32. The system of claim 1, wherein the electrons of multielectron atoms all exist as orbitspheres of discrete radii which are given by  $r_n$  of the radial Dirac delta function,  $\delta(r-r_n)$ .
  - 33. The system of claim 32, wherein electron orbitspheres may be spin paired or unpaired depending on the force balance which applies to each electron wherein the electron configuration is a minimum of energy.
  - 34. The system of claim 33, wherein the minimum energy configurations are given by solutions to Laplace's equation.
- 35. The system of claim 34, wherein the electrons of an atom with the same principal and 1 quantum numbers align parallel until each of the m 1 levels are occupied, and then pairing occurs until each of the m 1 levels contain paired

electrons.

5

10

- 36. The system of claim 35, wherein the electron configuration for one through twenty-electron atoms that achieves an energy minimum is: 1s < 2s < 2p < 3s < 3p < 4s.
- 37. The system of claim 36, wherein the corresponding force balance of the central centrifical, Coulombic, paramagnetic, magnetic, and diamagnetic forces for an electron configuration was derived for each n-electron atom that was solved for the radius of each electron.
- 38. The system of claim 37, wherein the central Coulombic force is that of a point charge at the origin since the electron charge-density functions are spherically symmetrical with a time dependence that is nonradiative.
- 39. The system of claim 38, wherein the ionization energies are obtained using the calculated radii in the determination of the Coulombic and any magnetic energies.
- 20 40. The system of claim 39, wherein the general equation for the radii of s electrons is given by

$$\frac{a_{0}\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}\pm a_{0}\left(\frac{\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}\right)^{2}}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}+\frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]Er_{m}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}$$

 $r_m$  in units of  $a_0$ 

where positive root must be taken in order that  $r_n > 0$ ;

Z is the nuclear charge, n is the number of electrons,

25  $r_m$  is the radius of the proceeding filled shell(s) given by

WO 2005/067678

PCT/US2005/000073

$$\frac{a_{0}\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)^{2}} + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]Er_{m}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}$$

$$= \frac{20\sqrt{3}\left(\frac{Z-n}{Z-(n-1)}\right)Er_{m}}{2}$$

r\_ in units of a

for the preceding s shell(s);

$$\frac{a_{0}}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)} \pm a_{0} + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_{3}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)}$$

r, in units of a

for the 2p shell, and

$$\frac{a_{0}}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)^{2}} \pm a_{0} + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}$$

 $r_{12}$  in units of  $a_0$ 

for the 3p shell;

5

the parameter A corresponds to the diamagnetic force,  $\mathbf{F}_{diamagnetic}$ :

$$\mathbf{F}_{diamagnetic} = -\frac{\hbar^2}{4m_e r_3^2 r_1} \sqrt{s(s+1)} \mathbf{i}_r;$$

the parameter  $\it B$  corresponds to the paramagnetic force,  $\it F_{\it mag\,2}$ :

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^2}{m_{J} r_A^2} \sqrt{s(s+1)} \mathbf{i}_r;$$

the parameter C corresponds to the diamagnetic force,  $\mathbf{F}_{\text{diamagnetic 3}}$ :

$$\mathbf{F}_{diamagnetic 3} = -\frac{1}{Z} \frac{8\hbar^2}{m_{f_{11}}^3} \sqrt{s(s+1)} \mathbf{i}_r;$$

the parameter D corresponds to the paramagnetic force,  $\mathbf{F}_{mag}$ :

5 
$$\mathbf{F}_{mag} = \frac{1}{4\pi c_2^2} \frac{1}{Z} \frac{\hbar^2}{m_e r^3} \sqrt{s(s+1)}$$
, and

the parameter E corresponds to the diamagnetic force,  $\mathbf{F}_{diamagnetic\ 2}$ , due to a relativistic effect with an electric field for  $r>r_n$ :

$$\mathbf{F}_{diamagnetic 2} = -\left[\frac{Z-3}{Z-2}\right] \frac{r_1 \hbar^2}{m_{r_3}^4} 10\sqrt{3/4} \mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic 2} = -\left[\frac{Z-11}{Z-10}\right] \left(1 + \frac{\sqrt{2}}{2}\right) \frac{r_{10} \hbar^2}{m_{e} r_{11}^4} 10\sqrt{s(s+1)} \mathbf{i}_r, \text{ and}$$

10 
$$\mathbf{F}_{diamagnetic 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)\frac{r_{18}\hbar^{2}}{m_{c}r_{n}^{4}}10\sqrt{s(s+1)}\mathbf{i}_{r}.$$

whereir Atom Type	n the parameters of a Electron Configuration		ing the 1s, 2 Orbital Arrangement of s Electrons (s state)	Diamag	and 4s of Parama g. Force Factor B		Para mag.	Force Factor
Neutral 1 e Atom	1 <i>s</i> ¹	<sup>2</sup> S <sub>1/2</sub> ~	1s	0	0	0	0	0
H Neutral 2 e Atom	1s <sup>2</sup>	¹S <sub>0</sub>	<u>↑</u> ↓ 1s	0	0	0	1	0
He Neutral 3 e Atom	2s <sup>1</sup>	<sup>2</sup> S <sub>1/2</sub>	<u>↑</u> 2s	1	0	0	0	0
Li Neutral 4 e Atom	$2s^2$	¹S <sub>0</sub>	<u>↑</u> ↓ 2s	1	0	0	1	0
11 e Atom	$1s^22s^22p^63s^1$	<sup>2</sup> S <sub>1/2</sub>	<u>↑</u> 3s	1	0	8	0	0
12 e Atom	$1s^22s^22p^63s^2$	<sup>1</sup> S <sub>0</sub>	<u>↑</u> ↓ 3s	1	3	12	1	0
19 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	<sup>2</sup> S <sub>1/2</sub>	<u>↑</u> 4s	2	0	12	0	0
K Neutral 20 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	<sup>1</sup> S <sub>0</sub>	<u>↑</u>	1	3	24	1	0
Ca 1 e Ion	1s1	$^{2}S_{1/2}$	1s	0	0	0	0	0
2 e lon	1s <sup>2</sup>	¹S <sub>0</sub>	<u>↑</u> ↓ 1s	0	0	0	1	0
3 e Ion	2 <i>s</i> ¹	<sup>2</sup> S <sub>1/2</sub>		1	0	0	0	1
4 e lon	2 <i>s</i> <sup>2</sup>	¹S <sub>0</sub>	<u>↑</u> 2s	1	0	0	1	1

WO 2005/067678

PCT/US2005/000073

11 e 
$$1s^2 2s^2 2p^6 3s^1$$
  ${}^2S_{1/2}$   $\frac{\uparrow}{3s}$  1 4 8 0  $1 + \frac{\sqrt{2}}{2}$ 

12 e  $1s^2 2s^2 2p^6 3s^2$   ${}^1S_0$   $\frac{\uparrow}{4s}$  1 6 0 0  $1 + \frac{\sqrt{2}}{2}$ 

19 e  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$   ${}^2S_{1/2}$   $\frac{\uparrow}{4s}$  3 0 24 0  $2 - \sqrt{2}$ 

20 e  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$   ${}^1S_0$   $\frac{\uparrow}{4s}$  2 0 24 0  $2 - \sqrt{2}$ 

- 41. The system of claim 40, with the radii,  $r_n$ , wherein the ionization energy for atoms having an outer s-shell are given by the negative of the electric energy,
- E(electric), given by:

$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_o r_n}$$

except that minor corrections due to the magnetic energy must be included in cases wherein the s electron does not couple to p electrons as given by

Ionization Energy (He) = 
$$-E(electric) + E(magnetic) \left(1 - \frac{1}{2} \left(\left(\frac{2}{3}\cos\frac{\pi}{3}\right)^2 + \alpha\right)\right)$$

Ionization Energy =  $-Electric Energy - \frac{1}{7}Magnetic Energy$ 10

$$E(ionization; Li) = \frac{(Z-2)e^2}{8\pi\epsilon_o r_3} + \Delta E_{mag}$$

$$= 5.3178 \ eV + 0.0860 \ eV = 5.4038 \ eV$$

15

$$= 5.3178 \ eV + 0.0860 \ eV = 5.4038 \ eV$$
 
$$E(Ionization) = E(Electric) + E_T$$
 
$$E(ionization; Be) = \frac{(Z-3)e^2}{8\pi\varepsilon_o r_4} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_4^3} + \Delta E_{mag}$$
 , and 
$$= 8.9216 \ eV + 0.03226 \ eV + 0.33040 \ eV = 9.28430 \ eV$$

$$E(Ionization) = -Electric Energy - \frac{1}{Z}Magnetic Energy - E_{\tau}.$$

The system of claim 41, wherein the radii and energies of the 2p electrons are 42. solved using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z-n)e^2}{4\pi\varepsilon_o r_n^2} \mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell+|m|)}{(2\ell+1)(\ell-|m|)} \frac{\hbar^2}{4m r_n^2 r_n} \sqrt{s(s+1)} \mathbf{i}_r$$

PCT/US2005/000073

$$\begin{aligned} \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^{2}}{m_{r}^{2} r_{3}^{2}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{4\hbar^{2}}{m_{r}^{2} r_{3}^{2}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^{2}}{m_{r}^{2} r_{3}^{2}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{diamagnetic 2} &= - \left[ \frac{Z-n}{Z-(n-1)} \right] \left( 1 - \frac{\sqrt{2}}{2} \right) \frac{r_{3}\hbar^{2}}{m_{r}r_{s}^{4}} 10 \sqrt{s(s+1)} \mathbf{i}_{r} , \end{aligned}$$

5 and the radii r<sub>3</sub> are given by

$$r_{4} = r_{3} = \frac{\left[\begin{array}{c} a_{0} \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right) \\ \left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right]}{\left(\left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)^{2}} + 4 \frac{\left[\frac{Z - 3}{Z - 2}\right] r_{1} 10 \sqrt{\frac{3}{4}}}{\left(\left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)}\right]}$$

r, in units of a

43. The system of claim 42, wherein the electric energy given by  $E(Ionization) = -Electric \ Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_a r_a}$ 

- gives the corresponding ionization energies.
- 44. The system of claim 43, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration  $1s^22s^22p^{n-4}$ , there are two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_1$  and  $r_2$
- 15 both given by:

10

$$r_1 = r_2 = a_o \left[ \frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_3$  and  $r_4$  both given by:

$$r_{4} = r_{3} = \frac{\left[\begin{array}{c} a_{0} \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right) \\ \left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right]}{\left(\left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)^{2} + 4 \frac{\left[\frac{Z - 3}{Z - 2}\right] r_{1} 10 \sqrt{\frac{3}{4}}}{\left(\left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)}\right]}$$

 $r_1$  in units of  $a_o$ 

and n-4 electrons in an orbitsphere with radius  $r_n$  given by

$$r_{n} = \frac{a_{0}}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{\frac{1}{2}}} + \frac{1}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)} + \frac{20\sqrt{3}\left(\left[\frac{Z - n}{Z - (n-1)}\right]\left(1 - \frac{\sqrt{2}}{2}\right)r_{3}\right)}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)};$$

r<sub>3</sub> in units of a<sub>0</sub>

the positive root must be taken in order that  $r_n > 0$ ;

the parameter  $\emph{A}$  corresponds to the diamagnetic force,  $\emph{\textbf{F}}_{\textit{diamagnetic}}$ :

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell + |m|)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^{2}}{4m_{e}r_{n}^{2}r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r};$$

and the parameter B corresponds to the paramagnetic force,  $\mathbf{F}_{mag\,2}$ :

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{f_{n}}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r},$$

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{f_{n}}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r}, \text{ and}$$

$$5 \quad \mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{f_{n}}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

wherein the parame Atom Type	eters of five th Electron Configuratio n	Ground		Diam agneti c Force	Para magn etic Force Facto r
Neutral 5 e Atom	$1s^22s^22p^1$	$^{2}P_{1/2}^{0}$	1 0 -1	2	0
Neutral 6 e Atom	$1s^22s^22p^2$	$^{3}P_{0}$	<u>↑</u> <u>↑</u>	<u>2</u> 3	0
Neutral 7 e Atom	$1s^22s^22p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ \hline 1 & 0 & -1 \end{array}$	$\frac{1}{3}$	1
Neutral 8 e Atom O	$1s^22s^22p^4$	$^{3}P_{2}$	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	1	2
Neutral 9 e Atom	$1s^22s^22p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ 1 & 0 & -1 & \end{array}$	<u>2</u> 3.	3
Neutral 10 e Atom Ne	$1s^22s^22p^6$	¹S <sub>0</sub>	$\begin{array}{ccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 & \\ \end{array}$	0	3
5 e lon	$1s^22s^22p^1$	$^{2}P_{1/2}^{0}$	1 0 -1	5 3	1
6 e lon	$1s^22s^22p^2$	$^{3}P_{0}$	$\begin{array}{c c} \uparrow & \uparrow & \\ \hline 1 & 0 & -1 \end{array}$	<u>5</u>	4
7 e Ion	$1s^22s^22p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ \hline 1 & 0 & -1 \end{array}$	$\frac{5}{3}$	6
8 e Ion	$1s^22s^22p^4$	$^{3}P_{2}$	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	<u>5</u>	6
9 e Ion	$1s^22s^22p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ \hline 1 & 0 & -1 & \end{array}$	<u>5</u>	9
10 e Ion	$1s^22s^22p^6$	<sup>1</sup> S <sub>0</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow & \downarrow \\ 1 & 0 & -1 & \end{array}$	<u>5</u>	12

WO 2005/067678

PCT/US2005/000073

45. The system of claim 44, wherein the ionization energy for the boron atom is given by

$$E(ionization; B) = \frac{(Z-4)e^2}{8\pi\varepsilon_o r_s} + \Delta E_{mag}$$

$$= 8.147170901 \ eV + 0.15548501 \ eV = 8.30265592 \ eV$$

The system of claim 44, wherein the ionization energies for the n-electron atoms having the radii,  $r_n$ , are given by the negative of the electric energy, E(electric), given by

$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_0 r_n}.$$

The system of claim 1, wherein the radii of the 3p electrons are given using the forces given by

$$F_{ele} = \frac{(Z - n)e^{2}}{4\pi\varepsilon_{o}r_{n}^{2}} \mathbf{i}_{r}$$

$$F_{diamagnetic} = -\sum_{m} \frac{(\ell + |m|)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^{2}}{4m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$
15 
$$F_{diamagnetic} = -\left(\frac{2}{3} + \frac{2}{3} + \frac{1}{3}\right) \frac{\hbar^{2}}{4m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r} = -\left(\frac{5}{3}\right) \frac{\hbar^{2}}{4m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$F_{mag2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$F_{mag2} = (4 + 4 + 4) \frac{1}{Z} \frac{\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$F_{mag2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$F_{mag2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$F_{mag2} = \frac{1}{Z} \frac{8\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$
and the radii  $r_{12}$  are given by

WO 2005/067678

PCT/US2005/000073

$$\frac{a_{0}}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)} \pm a_{0} \left(\frac{1}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}\right)^{2} + \frac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}$$

$$z_{12} = \frac{20\sqrt{3}\left(\frac{Z-12}{Z-11}\right)\left(1+\frac{\sqrt{2}}{2}\right)r_{10}}{2}$$

 $r_{10}$  in units of  $a_0$ 

48. The system of claim 47, wherein the ionization energies are given by electric energy given by:

5 
$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_0 r_n}$$
.

49. The system of claim 1, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>3s<sup>2</sup>3p<sup>n-12</sup>, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r<sub>1</sub> and r<sub>2</sub> both given by:

$$r_1 = r_2 = a_o \left[ \frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_3$  and  $r_4$  both given by:

### PCT/US2005/000073

$$r_{4} = r_{3} = \frac{\left[ \left( z - 3 \right) - \left( \frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_{1}} \right]}{\left[ \left( z - 3 \right) - \left( \frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_{1}} \right]^{2} + 4 \frac{\left[ \frac{z - 3}{z - 2} \right] r_{1} 10 \sqrt{\frac{3}{4}}}{\left( z - 3 \right) - \left( \frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_{1}} \right]}$$

 $r_1$  in units of  $a_o$  three sets of paired indistinguishable electrons in an orbitsphere with radius  $r_{10}$  given by:

$$r_{10} = \frac{a_0}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)^{\frac{1}{2}}} + \frac{1}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)} + \frac{20\sqrt{3}\left(\left[\frac{Z-10}{Z-9}\right]\left(1 - \frac{\sqrt{2}}{2}\right)r_3\right)}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)}$$

r<sub>3</sub> in units of a<sub>0</sub>

5 two indistinguishable spin-paired electrons in an orbitsphere with radius  $r_{12}$  given by:

PCT/US2005/000073

$$r_{12} = \frac{a_0}{\left[ (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right]^2} \pm a_0} + \frac{1}{\left[ (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right]} + \frac{20\sqrt{3} \left[ \left[ \frac{Z-12}{Z-11} \right] \left( 1 + \frac{\sqrt{2}}{2} \right) r_{10} \right)}{\left( (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right)}$$

 $r_{10}$  in units of  $a_0$ 

and n-12 electrons in a 3p orbitsphere with radius  $r_n$  given by

$$r_{n} = \frac{a_{0}}{\left[ (Z - (n-1)) - \left( \frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right]^{2}} + \frac{1}{\left[ (Z - (n-1)) - \left( \frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right]} + \frac{20\sqrt{3} \left[ \frac{Z - n}{Z - (n-1)} \right] \left( 1 - \frac{\sqrt{2}}{2} + \frac{1}{2} \right) r_{12}}{\left( (Z - (n-1)) - \left( \frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right)}$$

 $r_{12}$  in units of  $a_0$ 

where the positive root must be taken in order that  $r_n > 0$ ;

the parameter A corresponds to the diamagnetic force,  $\mathbf{F}_{diamagnetic}$ :

 $\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{\left(\ell + |m|\right)!}{\left(2\ell + 1\right)\left(\ell - |m|\right)!} \frac{\hbar^2}{4m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r \text{, and the parameter } B \text{ corresponds to}$ 

the paramagnetic force,  $\mathbf{F}_{mag 2}$ :

5

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{z} r_{n}^{2} r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag 2} = (4+4+4) \frac{1}{Z} \frac{\hbar^{2}}{m_{z} r_{n}^{2} r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r} = \frac{1}{Z} \frac{12\hbar^{2}}{m_{z} r_{n}^{2} r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$10 \quad \mathbf{F}_{mag 2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{z} r_{n}^{2} r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{z} r_{n}^{2} r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}, \text{ and}$$

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{8\hbar^{2}}{m_{z} r_{n}^{2} r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

Atom	the parameters of t Electron Configuration		hrough eighteen-ele Orbital Arrangement of 3p Electrons (3p state)	ctron ator Diamag netic Force Factor A	ns are Parama gnetic Force Factor B
13 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^{2}P_{1/2}^{0}$	1 0 -1	11 3	0
14 e Atom	$1s^22s^22p^63s^23p^2$	$^{3}P_{0}$	$\begin{array}{cccc} \uparrow & \uparrow & \\ \hline 1 & 0 & -1 \end{array}$	$\frac{7}{3}$	0
Si Neutral 15 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	<u>5</u> 3	2
16 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^4$	<sup>3</sup> P <sub>2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	<u>4</u> ·	1
17 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^5$	$^{2}P_{3/2}^{0}$	$ \begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array} $	$\frac{2}{3}$	2
Cl Neutral 18 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6$	<sup>1</sup> S <sub>0</sub>	$ \begin{array}{cccc} \uparrow & \uparrow & \downarrow & \uparrow \downarrow \\ 1 & 0 & -1 \end{array} $	$\frac{1}{3}$	4
<i>Ar</i> 13 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^{2}P_{1/2}^{0}$	$\begin{array}{c c} \uparrow & \hline 1 & 0 & -1 \end{array}$	<u>5</u> 3	12
14 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^2$	<sup>3</sup> P <sub>0</sub>	1 0 -1	$\frac{1}{3}$	16
15 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	0	24
16 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^4$	$^{3}P_{2}$	$\begin{array}{cccc} \uparrow & & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	$\frac{1}{3}$	24
17 e Ion	$1s^22s^22p^63s^23p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	2/3	32
18 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6$	¹S <sub>0</sub>	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	40

WO 2005/067678

50. The system of claim 49, wherein the ionization energies for the n-electron 3p atoms are given by electric energy given by:

$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_0 r_n}.$$

5 51. The system of claim 50, wherein the ionization energy for the aluminum atom is given by

$$E(ionization; Al) = \frac{(Z-12)e^2}{8\pi\epsilon_o r_{13}} + \Delta E_{mag}$$
  
= 5.95270 eV + 0.031315 eV = 5.98402 eV

10 52. A system of computing the nature of bound atomic and atomic ionic electrons from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration, 15

comprising:

20

25

processing means for processing and solving the equations for charge, mass, and current density functions of electron(s) in selected atoms or ions, wherein the equations are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration; and

- output means for outputting the solutions of the charge, mass, and current density functions of the atoms and atomic ions.
- 53. A method comprising the steps of;
- a.) inputting electron functions that are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration;
  - b.) inputting a trial electron configuration;
- c.) inputting the corresponding centrifugal, Coulombic, diamagnetic and paramagnetic forces.
- d.) forming the force balance equation comprising the centrifugal force equal to the sum of the Coulombic, diamagnetic and paramagnetic forces; 30
  - e.) solving the force balance equation for the electron radii;
  - f.) calculating the energy of the electrons using the radii and the corresponding electric and magnetic energies;
    - g.) repeating Steps a-f for all possible electron configurations, and

h.) outputting the lowest energy configuration and the corresponding electron radii for that configuration.

- 54. The method of claim 53, wherein the output is rendered using the electron functions.
  - 55. The method of claim 54, wherein the electron functions are given by at least one of the group comprising:

5

$$\rho(r,\theta,\phi,t) = \frac{e}{8\pi r^2} \left[ \delta(r-r_n) \right] \left[ Y_0^0(\theta,\phi) + Y_t^m(\theta,\phi) \right]$$

\$ ≠0

15

$$\rho(r,\theta,\phi,t) = \frac{e}{4\pi r^2} \left[\delta(r-r_n)\right] \left[Y_0^0(\theta,\phi) + \operatorname{Re}\left\{Y_t^m(\theta,\phi)e^{i\omega_n t}\right\}\right]$$

where  $Y_{\ell}^{m}(\theta,\phi)$  are the spherical harmonic functions that spin about the z-axis with angular frequency  $\omega_{n}$  with  $Y_{0}^{0}(\theta,\phi)$  the constant function.

Re  $\left\{Y_{\ell}^{m}(\theta,\phi)e^{i\omega_{\ell}}\right\} = P_{\ell}^{m}(\cos\theta)\cos\left(m\phi + \omega_{n}t\right)$  where to keep the form of the spherical harmonic as a traveling wave about the z-axis,  $\omega_{n} = m\omega_{n}$ .

56. The method of claim 55, wherein the forces are given by at least one of the group comprising:

25 
$$\mathbf{F}_{ele} = \frac{(Z - n)e^{2}}{4\pi\varepsilon_{o}r_{n}^{2}} \mathbf{i}_{r}$$

$$\mathbf{F}_{ele} = \frac{(Z - (n - 1))e^{2}}{4\pi\varepsilon_{o}r_{n}^{2}} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag} = \frac{1}{4\pi\varepsilon_{o}^{2}} \frac{1}{Z} \frac{\hbar^{2}}{m_{e}r^{3}} \sqrt{s(s + 1)}$$

$$\mathbf{F}_{diamagnetic} = -\frac{\hbar^{2}}{4m_{e}r_{o}^{2}r_{1}} \sqrt{s(s + 1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell + |m|)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^{2}}{4m_{e}r_{n}^{2}r_{1}} \sqrt{s(s + 1)} \mathbf{i}_{r}$$
30 
$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell + |m|)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^{2}}{4m_{e}r_{n}^{2}r_{12}} \sqrt{s(s + 1)} \mathbf{i}_{r}$$

$$\begin{split} \mathbf{F}_{diamagnetic} &= -\left(\frac{2}{3} + \frac{2}{3} + \frac{1}{3}\right) \frac{\hbar^2}{4m_f r_{12}^2} \sqrt{s(s+1)} \mathbf{i}_r = -\left(\frac{5}{3}\right) \frac{\hbar^2}{4m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{diamagnetic 2} &= -\left[\frac{Z-3}{Z-2}\right] \frac{r_1 \hbar^2}{m_f r_3^4} 10 \sqrt{3/4} \mathbf{i}_r \\ \mathbf{F}_{diamagnetic 2} &= -\left[\frac{Z-n}{Z-(n-1)}\right] \left(1 - \frac{\sqrt{2}}{2}\right) \frac{r_1 \hbar^2}{m_e r_n^4} 10 \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{diamagnetic 2} &= -\left[\frac{Z-11}{Z-10}\right] \left(1 + \frac{\sqrt{2}}{2}\right) \frac{r_1 h^2}{m_e r_1^4} 10 \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{diamagnetic 2} &= -\left[\frac{Z-n}{Z-(n-1)}\right] \left(1 - \frac{\sqrt{2}}{2} + \frac{1}{2} - \frac{\sqrt{2}}{2} + \frac{1}{2}\right) \frac{r_1 h^2}{m_f r_n^4} 10 \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{diamagnetic 3} &= -\frac{1}{Z} \frac{8 \hbar^2}{m_e r_{11}^3} \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_3} \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{mag 2} &= \left(4 + 4 + 4\right) \frac{1}{Z} \frac{\hbar^2}{m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{4 \hbar^2}{m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r, \text{ and} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{8 \hbar^2}{m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r, \text{ and} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{8 \hbar^2}{m_e r_n^2 r_{12}} \sqrt{s(s+1)} \mathbf{i}_r. \end{split}$$

15 57. The method of claim 53, wherein the radii are given by at least one of the group comprising:

$$r_1 = r_2 = a_o \left[ \frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

WO 2005/067678

#### PCT/US2005/000073

$$a_{0}\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right) = \frac{\left(1-\frac{\sqrt{\frac{3}{4}}}{Z}\right)^{2}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)^{2}} + 4\frac{\left[\frac{Z-3}{Z-2}\right]r_{1}10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)^{2}} + 4\frac{\left[\frac{Z-3}{Z-2}\right]r_{1}10\sqrt{\frac{3}{4}}}{\left((Z-3)-\left(\frac{1}{4}-\frac{1}{Z}\right)\frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)^{2}}$$

r, in units of a

$$\frac{a_{0}}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{\frac{1}{2}}} \pm a_{0} \left(\frac{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{\frac{1}{2}}}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)} + \frac{20\sqrt{3}\left(\left(\frac{Z-n}{Z-(n-1)}\right)\left(1-\frac{\sqrt{2}}{2}\right)r_{3}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)}$$

 $\frac{a_{0}}{\left((Z-9)-\left(\frac{5}{24}-\frac{6}{Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{2}} \pm a_{0} \left(\frac{1}{\left((Z-9)-\left(\frac{5}{24}-\frac{6}{Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{2}} + \frac{20\sqrt{3}\left(\left[\frac{Z-10}{Z-9}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_{3}\right)}{\left((Z-9)-\left(\frac{5}{24}-\frac{6}{Z}\right)\frac{\sqrt{3}}{r_{3}}\right)}\right)$ 

r<sub>3</sub> in units of a<sub>0</sub>

$$r_{11} = \frac{a_0 \left(1 + \frac{8}{Z} \sqrt{\frac{3}{4}}\right)}{(Z - 10) - \frac{\sqrt{\frac{3}{4}}}{4r_{10}}}, \ r_{10} \ in \ units \ of \ a_0$$

$$\frac{a_{0}}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)^{2}}\pm a_{0}} + \frac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}$$

$$= \frac{20\sqrt{3}\left(\left[\frac{Z-12}{Z-11}\right]\left(1+\frac{\sqrt{2}}{2}\right)r_{10}\right)}{\left((Z-11)-\left(\frac{1}{8}-\frac{3}{Z}\right)\frac{\sqrt{3}}{r_{10}}\right)}$$

$$\frac{a_0}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)^{\frac{1}{2}}} \pm a_0} + \frac{1}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)} \left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)} + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}$$

$$a_{0}\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right) = \begin{bmatrix} \left(1+(C-D)\frac{\sqrt{3}}{2Z}\right) & \left(1+(C-D)\frac{\sqrt{3}}{2Z}\right) & \left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right) & \left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right) & \\ + \left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r$$

5 58. The method of claim 53, wherein the electric energy of each electron of radius  $r_n$  is given by at least one of the group comprising:

r, in units of a

$$E(electric) = -\frac{(Z - (n-1))e^2}{8\pi\varepsilon_o r_n}$$

$$Ionization\ Energy(He) = -E(electric) + E(magnetic) \left(1 - \frac{1}{2} \left(\frac{2}{3}\cos\frac{\pi}{3}\right)^2 + \alpha\right)$$

Ionization Energy = 
$$-Electric Energy - \frac{1}{Z}Magnetic Energy$$

$$E(Ionization) = -Electric Energy - \frac{1}{Z}Magnetic Energy - E_T$$

$$E(ionization; Li) = \frac{(Z-2)e^2}{8\pi\varepsilon_o r_3} + \Delta E_{mag}$$

$$= 5.3178 \ eV + 0.0860 \ eV = 5.4038 \ eV$$

$$E(ionization; B) = \frac{(Z-4)e^2}{8\pi\varepsilon_o r_5} + \Delta E_{mag}$$

$$= 8.147170901 \ eV + 0.15548501 \ eV = 8.30265592 \ eV$$

$$E(ionization; Be) = \frac{(Z-3)e^2}{8\pi\varepsilon_o r_4} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_4^3} + \Delta E_{mag}$$

$$= 8.9216 \ eV + 0.03226 \ eV + 0.33040 \ eV = 9.28430 \ eV$$

$$E(ionization; Na) = -Electric Energy = \frac{(Z-10)e^2}{8\pi\varepsilon_o r_1} = 5.12592 \ eV$$

5

59. The method of claim 53, wherein the radii of s electrons are given by

$$a_{0}\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right) = \left(\frac{\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)^{2}} \pm a_{0}\left(\frac{\left(Z-(n-1)\right)-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)^{2}}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)} + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]Er_{m}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}$$

 $r_m$  in units of  $a_0$ 

where positive root must be taken in order that  $r_n > 0$ ;

Z is the nuclear charge, n is the number of electrons,  $r_m$  is the radius of the proceeding filled shell(s) given by

$$\frac{a_{0}\left(1+(C-D)\frac{\sqrt{3}}{2Z}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)^{\pm}a_{0}} + \frac{20\sqrt{3}\left(\left[\frac{Z-n}{Z-(n-1)}\right]Er_{m}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{m}}\right)}$$

for the preceding s shell(s);

$$\frac{a_{0}}{\left[(Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{\pm}a_{0}} + \frac{20\sqrt{3}\left[\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}\right)r_{3}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)}$$

for the 2p shell, and

$$\frac{a_{0}}{\left[(Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)^{2}} \pm a_{0} + \frac{20\sqrt{3}\left[\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)r_{12}\right)}{\left((Z-(n-1))-\left(\frac{A}{8}-\frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{12}}\right)}$$

r<sub>12</sub> in units of a<sub>0</sub>

for the 3p shell;

5

the parameter  $\emph{A}$  corresponds to the diamagnetic force,  $\mathbf{F}_{\textit{diamagnetic}}$ :

$$\mathbf{F}_{diamagnetic} = -\frac{\hbar^2}{4m_r r_s^2 r_i} \sqrt{s(s+1)} \mathbf{i}_r;$$

the parameter  $\it B$  corresponds to the paramagnetic force,  $\it F_{mag\,2}$ :

WO 2005/067678

PCT/US2005/000073

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^2}{m r_1 r_4^2} \sqrt{s(s+1)} \mathbf{i}_r$$
;

the parameter C corresponds to the diamagnetic force,  $\mathbf{F}_{diamagnetic\ 3}$ :

$$\mathbf{F}_{diamagnetic 3} = -\frac{1}{Z} \frac{8\hbar^2}{m r_{13}^3} \sqrt{s(s+1)} \mathbf{i}_r;$$

the parameter D corresponds to the paramagnetic force,  $\mathbf{F}_{mag}$ :

5 
$$\mathbf{F}_{mag} = \frac{1}{4\pi r_2^2} \frac{1}{Z} \frac{\hbar^2}{m_e r^3} \sqrt{s(s+1)}$$
, and

the parameter E corresponds to the diamagnetic force,  $\mathbf{F}_{diamagnetic 2}$ , due to a relativistic effect with an electric field for  $r > r_n$ :

$$\mathbf{F}_{diamagnetic 2} = -\left[\frac{Z-3}{Z-2}\right] \frac{r_i \hbar^2}{m_e r_3^4} 10\sqrt{3/4} \mathbf{i}_r$$

$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-11}{Z-10}\right] \left(1 + \frac{\sqrt{2}}{2}\right) \frac{r_{10}\hbar^2}{m_e r_{11}^4} 10\sqrt{s(s+1)}\mathbf{i}_r$$
, and

10 
$$\mathbf{F}_{diamagnetic\ 2} = -\left[\frac{Z-n}{Z-(n-1)}\right]\left(1-\frac{\sqrt{2}}{2}+\frac{1}{2}-\frac{\sqrt{2}}{2}+\frac{1}{2}\right)\frac{r_1s\hbar^2}{m_er_n^4}10\sqrt{s(s+1)}\mathbf{i}_r.$$

wherein Atom Type	the parameters of a Electron Configuration		Orbital	Dia mag Forc e	Para mag Forc	Dia mag Forc e	Para mag Forc e	Diama
Neutral 1 e Atom	1s¹	<sup>2</sup> S <sub>1/2</sub>	1s	0	0	0	0	0
H Neutral 2 e Atom	1s <sup>2</sup>	¹S <sub>0</sub>	↑↓ ls	0	0	0	1	0
He Neutral 3 e Atom	2s <sup>1</sup>	<sup>2</sup> S <sub>1/2</sub>	<u>↑</u> 2s	1	0	0	0	0
Li Neutral 4 e Atom	2s <sup>2</sup>	¹S <sub>0</sub>	<u>↑</u> ↓ 2s	1	0	0	1	0
11 e Atom	$1s^22s^22p^63s^1$	<sup>2</sup> S <sub>1/2</sub>	<u>↑</u> 3s	1	0	8	0	0
12 e Atom	$1s^22s^22p^63s^2$	¹S <sub>0</sub>	<u>↑</u> ↓ 3s	1	3	12	1	0
Mg Neutral 19 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	<sup>2</sup> S <sub>1/2</sub>	<u>↑</u> 4s	2	0	12	0	0
20 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	¹S <sub>0</sub>	<u>↑</u> ↓ 4s	1	3	24	1	0
Ca 1 e Ion	1s <sup>1</sup>	<sup>2</sup> S <sub>1/2</sub>	1s	0	0	0	0	0
2 e Ion	1s <sup>2</sup>	<sup>1</sup> S <sub>0</sub>	1s	0	0	0	1	0
3 e lon	2 <i>s</i> ¹	<sup>2</sup> S <sub>1/2</sub>		1	0	0	0	1

- 60. The method of claim 59, with the radii,  $r_n$ , wherein the ionization energy for atoms having an outer s-shell are given by the negative of the electric energy.
- 5 *E*(*electric*), given by:

$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_0 r_0}$$

except that minor corrections due to the magnetic energy must be included in cases wherein the s electron does not couple to p electrons as given by

Ionization Energy(He) = 
$$-E(electric) + E(magnetic) \left(1 - \frac{1}{2} \left( \left( \frac{2}{3} \cos \frac{\pi}{3} \right)^2 + \alpha \right) \right)$$

Ionization Energy =  $-Electric Energy - \frac{1}{7}Magnetic Energy$ 10

$$E(ionization; Li) = \frac{(Z-2)e^2}{8\pi\epsilon_o r_3} + \Delta E_{mag}$$

$$= 5.3178 \ eV + 0.0860 \ eV = 5.4038 \ eV$$

$$E(Ionization) = E(Electric) + E_T$$

$$E(ionization; Be) = \frac{(Z-3)e^2}{8\pi\epsilon_o r_4} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r_4^3} + \Delta E_{mag}$$

$$= 8.9216 \ eV + 0.03226 \ eV + 0.33040 \ eV = 9.28430 \ eV$$

$$E(Ionization) = -Electric Energy - \frac{1}{Z}Magnetic Energy - E_T.$$

61. The method of claim 53, wherein the radii and energies of the 2p electrons are solved using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z - n)e^2}{4\pi\varepsilon_o r_n^2} \,\mathbf{i}_r$$

15

WO 2005/067678

$$\begin{aligned} \mathbf{F}_{diamagnetic} &= -\sum_{m} \frac{\left(\ell + |m|\right)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^{2}}{4m r_{n}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^{2}}{m r_{n}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{4\hbar^{2}}{m r_{n}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{mag 2} &= \frac{1}{Z} \frac{\hbar^{2}}{m r_{n}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r} \\ \mathbf{F}_{mag 2} &= -\left[\frac{Z-n}{Z-(n-1)}\right] \left(1 - \frac{\sqrt{2}}{2}\right) \frac{r_{3}\hbar^{2}}{m_{e} r_{n}^{4}} 10\sqrt{s(s+1)} \mathbf{i}_{r}, \\ \mathbf{and the radii} \ r_{3} \ \text{ are given by} \end{aligned}$$

$$r_{4} = r_{3} = \frac{\left( \frac{1 - \sqrt{\frac{3}{4}}}{2} \right)}{\left( (Z - 3) - \left( \frac{1}{4} - \frac{1}{Z} \right) \sqrt{\frac{3}{4}} \right)} \left( \frac{\left( \frac{1 - \sqrt{\frac{3}{4}}}{2} \right)^{2}}{\left( (Z - 3) - \left( \frac{1}{4} - \frac{1}{Z} \right) \sqrt{\frac{3}{4}} \right)^{2}} + 4 \frac{\left[ \frac{Z - 3}{Z - 2} \right] r_{1} 10 \sqrt{\frac{3}{4}}}{\left( (Z - 3) - \left( \frac{1}{4} - \frac{1}{Z} \right) \sqrt{\frac{3}{4}} \right)} \right)}$$

 $r_i$  in units of  $a_o$ 

62. The method of claim 61, wherein the electric energy given by

10 
$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_o r_n}$$

gives the corresponding ionization energies.

63. The method of claim 53, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration  $1s^2 2s^2 2 p^{n-4}$ , there are two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_1$  and  $r_2$  both given by:

$$r_1 = r_2 = a_o \left[ \frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_3$  and  $r_4$  both given by:

$$r_{4} = r_{3} = \frac{\left| \begin{array}{c} a_{0} \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right) \\ \left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}} \right|}{\left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right)^{2} + 4 \left(\frac{\left[\frac{Z - 3}{Z - 2}\right] r_{1} 10 \sqrt{\frac{3}{4}}}{\left(Z - 3\right) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}} \right)}{2} \right|$$

 $r_1$  in units of  $a_o$ 

5 and n-4 electrons in an orbitsphere with radius  $r_n$  given by

$$r_{n} = \frac{a_{0}}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)^{\pm} a_{0}} + \frac{1}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)} + \frac{20\sqrt{3}\left(\left[\frac{Z - n}{Z - (n-1)}\right]\left(1 - \frac{\sqrt{2}}{2}\right)r_{3}\right)}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z}\right)\frac{\sqrt{3}}{r_{3}}\right)};$$

r, in units of a

the positive root must be taken in order that  $r_n > 0$ ;

the parameter A corresponds to the diamagnetic force,  $\mathbf{F}_{\text{diamagnetic}}$ :

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell + |m|)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^2}{4m_{\ell}r_n^2 r_3} \sqrt{s(s+1)} \mathbf{i}_r;$$
 and the parameter  $B$  corresponds to the paramagnetic force,  $\mathbf{F}_{mag 2}$ :

$$\mathbf{F}_{mag2} = \frac{1}{Z} \frac{\hbar^2}{m_c r_n^2 r_3} \sqrt{s(s+1)} \mathbf{i}_r,$$

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{r} r_{n}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r}, \text{ and}$$

$$5 \quad \mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{r} r_{n}^{2} r_{3}} \sqrt{s(s+1)} \mathbf{i}_{r}.$$

5 
$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^2}{m_s r_n^2 r_1} \sqrt{s(s+1)} \mathbf{i}_r$$

wherein the parameters of five through ten-electron atoms are  Atom Type Electron Ground Orbital Diam Para								
Alom Type	Configuratio n		Arrangement	agnet c Force Facto r	i magn etic Force Facto r			
				A	В			
Neutral 5 e Atom  B	$1s^22s^22p^1$	$^{2}P_{1/2}^{0}$	$\frac{\uparrow}{1} {0} {-1}$	2	0			
Neutral 6 e Atom C	$1s^22s^22p^2$	$^{3}P_{0}$	$\begin{array}{c c} \uparrow & \uparrow & \\ \hline 1 & 0 & -1 \end{array}$	$\frac{2}{3}$	0			
Neutral 7 e Atom N	$1s^22s^22p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ \hline 1 & 0 & -1 \end{array}$	<u>1</u> 3	1			
Neutral 8 e Atom O	$1s^22s^22p^4$	<sup>3</sup> P <sub>2</sub>	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	1	2			
Neutral 9 e Atom	$1s^22s^22p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ 1 & 0 & -1 & \end{array}$	$\frac{2}{3}$	3			
Neutral 10 e Atom Ne	$1s^22s^22p^6$	<sup>1</sup> S <sub>0</sub>	$\begin{array}{ccc} \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	0	3			
5 e Ion	$1s^22s^22p^1$	$^{2}P_{1/2}^{0}$	1 0 -1	<u>5</u>	1			
6 e Ion	$1s^22s^22p^2$	$^{3}P_{0}$	1 0 -1	5 3	4			
7 e lon	$1s^22s^22p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	<u>5</u>	6			
8 e Ion	$1s^22s^22p^4$	<sup>3</sup> P <sub>2</sub>	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	<u>5</u>	6			
9 e Ion	$1s^22s^22p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ 1 & 0 & -1 & \\ \end{array}$	<u>5</u>	9			
10 e Ion	$1s^22s^22p^6$	¹S <sub>0</sub>	$\begin{array}{ccc} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow \\ 1 & 0 & -1 & & \\ \end{array}$	<u>5</u>	12			

64. The method of claim 63, wherein the ionization energy for the boron atom is given by

$$E(ionization; B) = \frac{(Z-4)e^2}{8\pi\epsilon_o r_5} + \Delta E_{mag}$$

$$= 8.147170901 \ eV + 0.15548501 \ eV = 8.30265592 \ eV$$

5 65. The method of claim 63, wherein the ionization energies for the n-electron atoms having the radii,  $r_n$ , are given by the negative of the electric energy,

E(electric), given by

$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_0 r_n}.$$

10 66. The method of claim 53, wherein the radii of the 3p electrons are given using the forces given by

$$\mathbf{F}_{ele} = \frac{(Z - n)e^{2}}{4\pi\varepsilon_{o}r_{n}^{2}} \mathbf{i}_{r}$$

$$\mathbf{F}_{diamagnetic} = -\sum_{m} \frac{(\ell + |m|)!}{(2\ell + 1)(\ell - |m|)!} \frac{\hbar^{2}}{4m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{diamagnetic} = -\left(\frac{2}{3} + \frac{2}{3} + \frac{1}{3}\right) \frac{\hbar^{2}}{4m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r} = -\left(\frac{5}{3}\right) \frac{\hbar^{2}}{4m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$15 \quad \mathbf{F}_{mag2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag2} = (4 + 4 + 4) \frac{1}{Z} \frac{\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r} = \frac{1}{Z} \frac{12\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag2} = \frac{1}{Z} \frac{8\hbar^{2}}{m_{c}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

20 and the radii  $r_{12}$  are given by

$$r_{12} = \frac{a_0}{\left[ (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right]^2 + \frac{20\sqrt{3} \left[ \frac{Z-12}{Z-11} \right] \left(1 + \frac{\sqrt{2}}{2}\right) r_{10}}{\left( (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right)}$$

 $r_{10}$  in units of  $a_0$ 

67. The method of claim 66, wherein the ionization energies are given by electric energy given by:

5 
$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_0 r_n}$$
.

68. The method of claim 53, wherein for each n-electron atom having a central charge of Z times that of the proton and an electron configuration  $1s^22s^22p^63s^23p^{n-12}$ , there are two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_1$  and  $r_2$  both given by:

$$r_1 = r_2 = a_o \left[ \frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right]$$

two indistinguishable spin-paired electrons in an orbitsphere with radii  $r_3$  and  $r_4$  both given by:

PCT/US2005/000073

$$r_{4} = r_{3} = \frac{\left[\begin{array}{c} a_{0} \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right) \\ \left((Z - 3) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right) \\ \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right)^{2} \\ \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z}\right)^{2} + 4 \left(\frac{\left[\frac{Z - 3}{Z - 2}\right]r_{1}10\sqrt{\frac{3}{4}}}{\left((Z - 3) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)}\right) \\ \left((Z - 3) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)^{2} + 4 \left((Z - 3) - \left(\frac{1}{4} - \frac{1}{Z}\right) \frac{\sqrt{\frac{3}{4}}}{r_{1}}\right)\right)$$

 $r_1$  in units of  $a_o$  three sets of paired indistinguishable electrons in an orbitsphere with radius  $r_{10}$  given by:

$$r_{10} = \frac{a_0}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)} \pm a_0} + \frac{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)\right)^2}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z}\right)\frac{\sqrt{3}}{r_3}\right)}$$

 $r_3$  in units of  $a_0$ 

5 two indistinguishable spin-paired electrons in an orbitsphere with radius  $r_{12}$  given by:

$$r_{12} = \frac{a_0}{\left[ (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right]} \pm a_0} + \frac{\left[ \left( (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right) \right]}{\left[ (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right]} + \frac{20\sqrt{3} \left[ \left[ \frac{Z-12}{Z-11} \right] \left( 1 + \frac{\sqrt{2}}{2} \right) r_{10} \right)}{\left[ (Z-11) - \left(\frac{1}{8} - \frac{3}{Z}\right) \frac{\sqrt{3}}{r_{10}} \right)}$$

and n-12 electrons in a 3p orbitsphere with radius  $r_n$  given by

$$r_{n} = \frac{a_{0}}{\left[ (Z - (n-1)) - \left( \frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right]^{2}} \pm a_{0}} + \frac{1}{\left[ (Z - (n-1)) - \left( \frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right]} + \frac{20\sqrt{3} \left[ \left[ \frac{Z - n}{Z - (n-1)} \right] \left( 1 - \frac{\sqrt{2}}{2} + \frac{1}{2} \right) r_{12} \right)}{\left( (Z - (n-1)) - \left( \frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right)}$$

 $r_{12}$  in units of  $a_0$ 

where the positive root must be taken in order that  $r_n > 0$ ;

the parameter A corresponds to the diamagnetic force,  $\mathbf{F}_{\textit{diamagnetic}}$ :

 $\mathbf{F}_{diamagnetic} = -\sum_{r} \frac{(\ell + |m|)!}{(2\ell + 1)!(\ell - |m|)!} \frac{\hbar^2}{4m r_c^2 r_c} \sqrt{s(s+1)} \mathbf{i}_r$ , and the parameter B corresponds to the paramagnetic force,  $\mathbf{F}_{mag,2}$ :

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{\hbar^{2}}{m_{e}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag 2} = (4+4+4) \frac{1}{Z} \frac{\hbar^{2}}{m_{e}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r} = \frac{1}{Z} \frac{12\hbar^{2}}{m_{e}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$10 \quad \mathbf{F}_{mag 2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{e}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{4\hbar^{2}}{m_{e}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}, \text{ and}$$

$$\mathbf{F}_{mag 2} = \frac{1}{Z} \frac{8\hbar^{2}}{m_{e}r_{n}^{2}r_{12}} \sqrt{s(s+1)} \mathbf{i}_{r}$$

15

wherein the parameters of thirteen to eighteen-electron atoms are

PCT/US2005/000073

# WO 2005/067678

Atom Type	Electron Configuration	Ground State Term	Orbital Arrangement of 3p Electrons (3p state)	Diamag netic Force Factor	Parama gnetic Force Factor B
13 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^{2}P_{1/2}^{0}$	1 0 -1	11 3	0
14 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^2$	$^{3}P_{0}$	1 0 -1	$\frac{7}{3}$	0
15 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^3$	$^{4}S_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ \hline 1 & 0 & -1 \end{array}$	<u>5</u> 3	2
P Neutral 16 e Atom S	$1s^2 2s^2 2p^6 3s^2 3p^4$	<sup>3</sup> P <sub>2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	4/3	1
Neutral 17 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \uparrow & \downarrow & \uparrow \\ 1 & 0 & -1 \end{array}$	$\frac{2}{3}$	2
18 e Atom	$1s^2 2s^2 2p^6 3s^2 3p^6$	<sup>1</sup> S <sub>0</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow & \downarrow \\ 1 & 0 & -1 & \end{array}$	$\frac{1}{3}$	4
Ar 13 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^1$	$^{2}P_{1/2}^{0}$	1 0 -1	<u>5</u> 3	12
14 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^2$	$^{3}P_{0}$	$\frac{\uparrow}{1}$ $\frac{\uparrow}{0}$ ${-1}$	1/3	16
15 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^3$	<sup>4</sup> S <sub>3/2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ \hline 1 & 0 & -1 \end{array}$	0	24
16 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^4$	<sup>3</sup> P <sub>2</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow \\ \hline 1 & 0 & -1 \end{array}$	1/3	24
17 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^5$	$^{2}P_{3/2}^{0}$	$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$	$\frac{2}{3}$	32
18 e Ion	$1s^2 2s^2 2p^6 3s^2 3p^6$	¹S <sub>0</sub>	$\begin{array}{cccc} \uparrow & \uparrow & \downarrow & \uparrow \downarrow \\ 1 & 0 & -1 & \end{array}$	0	40

5

69. The method of claim 68 wherein the ionization energies for the n-electron 3p atoms are given by electric energy given by:

$$E(Ionization) = -Electric Energy = \frac{(Z - (n-1))e^2}{8\pi\varepsilon_o r_n}.$$

70. The method of claim 68 wherein the ionization energy for the aluminum atom is given by

$$E(ionization; Al) = \frac{(Z-12)e^2}{8\pi\epsilon_o r_{13}} + \Delta E_{mag}$$

$$= 5.95270 \ eV + 0.031315 \ eV = 5.98402 \ eV$$